
Astrochemistry and Observations

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1 Introduction

The past few years has seen dramatic improvements in our ability to extract chemical information from molecular line observations. These advances have been driven by new observational platforms and techniques. In the following I will outline the various methods and uncertainties in computing chemical information from observations across the spectrum of star formation activity (from diffuse clouds, to star-forming cores, to molecular outflows). I will show how improved chemical knowledge can be used to place stronger constraints on theoretical astrochemical models, but also open new avenues in the use of molecular emission to examine the physics of molecular clouds and star formation.

2 Diffuse Cloud Chemistry

Diffuse clouds are transition objects between the low density atomic medium and the higher density molecular phase. The allure of diffuse clouds is twofold. First they are generally, but not exclusively, studied via absorption lines. For absorption lines the conversion of equivalent width to column density is fairly straightforward and requires little information regarding source structure. In contrast, knowledge of the density and temperature structure is often needed to obtain column densities from emission lines. Thus chemical abundances derived from absorption lines can be considered more reliable. Second, these objects present rather simple laboratories to study basic physical and chemical processes.

Over the past decade studies of diffuse cloud chemistry through absorption lines has received significant attention in a series of papers by Lucas and Liszt (see Liszt & Lucas 2002 and references therein). In Figure 1 I provide a sample of this work showing detections of HCO^+ ($J=1-0$) and CS ($J=2-1$) in absorption in several line of sight clouds. To study basic chemical processes

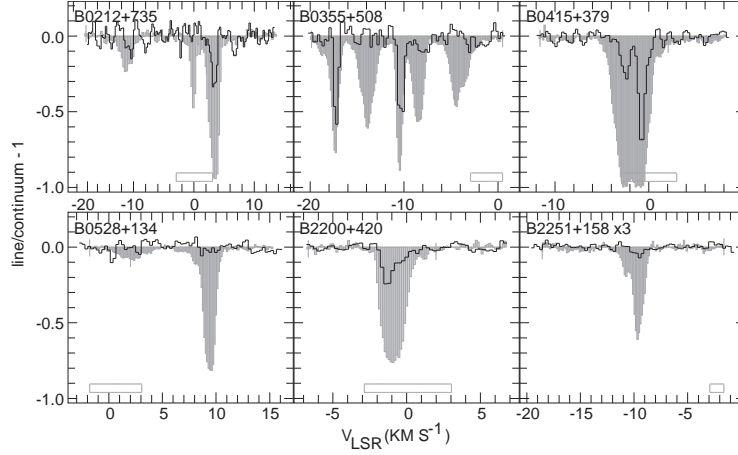


Fig. 1. CS J=2–1 (solid line) and HCO⁺ J=1–0 (grey overlay) absorption spectra towards 6 quasars. Taken from Lucas & Liszt (2002).

these investigations are able to observe the various species that constitute simple self-contained chemical networks. For instance, the network that creates CO in diffuse gas is believed to be: $C^+ + OH \rightarrow HCO^+$, followed by $HCO^+ + e \rightarrow CO + H$. Lucas & Liszt (2000) find that the column density of HCO⁺ is capable of accounting for the observed column density of CO. However, the measured abundances of C⁺ and OH are not high enough to account for observed HCO⁺. Thus either our understanding of ion-molecule gas phase chemistry is incorrect or diffuse clouds are not just “simple” laboratories. Indeed other more exotic non-thermal chemical processes have been invoked to overcome these failings (Zsargo & Federman 2003; Flower & Pineau des Forêts 1998).

3 Chemistry and Star Formation

The most significant recent advance in astrochemical studies of star-forming cores is the development of new techniques that move beyond line of sight average abundances, towards an examination of chemical structure as a function of depth. This is possible via new instrument capabilities which have provided images of the dust continuum emission, or information regarding the spatial distribution of dust absorption. This information has been gleaned through a variety of methods extending from 1.3mm and sub-mm continuum emission images (low-mass star-forming cores: André et al. 2000, Shirley et al. 2001; high-mass star-forming cores: van der Tak et al. 2000, Hatchell and van der Tak 2003), to images of dust absorption against the galactic mid-IR background (Bacmann et al. 2000), and near-IR extinction mapping (Alves, Lada, & Lada 2001).

Since the dust column density and mass is correlated with the H_2 column density and mass (Hildebrand 1983; Gordon 1995), these observations provide the clearest information to date on the column and volume density distribution of H_2 molecules. This significantly aids the molecular observations in two ways. (1) By indirectly confirming the location of the H_2 density and column density peak and, (2) by providing the density profile which helps to unravel the similar effects of density and abundance on excitation.

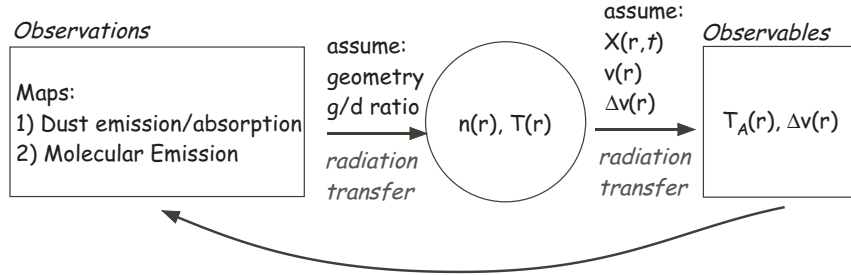


Fig. 2. Flow chart describing the iterative procedure used to determine abundance structure with depth. The abundance profile can either be assumed or predicted via a chemical model, in which case it can be time dependent.

In Figure 2 we present a flow chart that outlines this new iterative method to derive abundances. A key to this process is that spatial information is important for observations of both dust and gas. The first phase involves using dust observations to constrain core physical properties, typically the radial density profile.¹ At this point there are 2 methods that can be used to examine the abundance structure; both adopting spherical geometry.

(1) In the first method the density and temperature profile², and an assumed abundance profile are used as inputs to a radiative transfer model. The radiation transfer codes adopt either accelerated lambda iteration or Monte-Carlo methods. The results from this process are predictions of the emission spectra as a function of position, which can be compared directly to observations. An iterative procedure then determines the abundance profile (see van der Tak et al. 2000; Schreyer et al 2002; Tafalla et al 2002, 2003; Caselli et al 2002; Jorgensen et al. 2002; di Francesco et al. 2003; and Lee et al 2003). (2) The second method uses a chemical model (using the same density profile for the chemical and radiative transfer models) to predict the abundance profile. The abundance profile is then used as input to the radiative transfer producing observable quantities, which can be iterated by changing the parameters

¹ For cores with embedded stars the dust spectral energy distribution is used to estimate the radial temperature profile.

² Along with assumed profiles for radial velocity gradient and velocity dispersion.

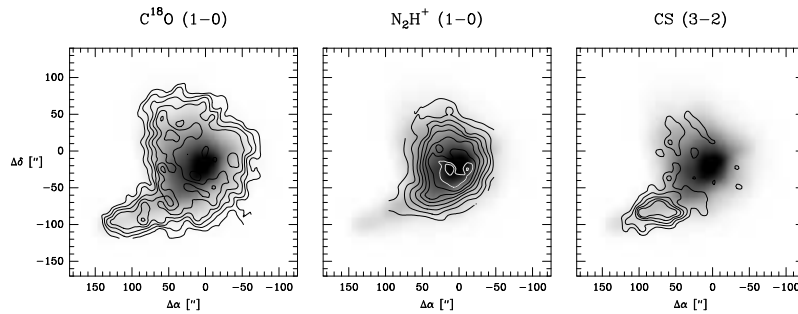


Fig. 3. The observed emission distribution of visual extinction or total column density (gray scale) in the B68 dark cloud. Contours are integrated emission maps of C^{18}O (left-hand panel), N_2H^+ (middle), and CS (right-hand panel). The N_2H^+ contours are reversed in color near the central peak to show the distribution in the center over the extinction distribution. The emission distributions illustrate sequence of increasing molecular depletion from CS , to C^{18}O , and even N_2H^+ (Bergin et al. 2002; Lada et al. 2003).

in the chemical model or by looking at the time-dependence (Bergin et al. 2002; Doty et al. 2002).

In the following we briefly discuss examples for pre-stellar cores and for sources which contain embedded sources.

3.1 Chemistry in Pre-Stellar Cores

A representative pre-stellar core is the dark cloud B68 where the centrally concentrated H_2 distribution is traced through a map of dust visual extinction (Alves, Lada, and Lada 2001). In Figure 3 we present the B68 A_V map along with a series of molecular emission maps. In this core we see that the N_2H^+ emission peaks in a shell partially surrounding the peak of dust extinction. Moreover, the N_2H^+ peaks inside the much larger C^{18}O emission hole, which itself lies inside the CS emission depression.

Figure 4 presents the analysis of the N_2H^+ and C^{18}O emission, which used a gas-grain chemical model linked to a Monte-Carlo radiative transfer code (Bergin et al. 2002). If the emission is in LTE and optically thin then the integrated emission from a source with constant abundance would appear as a straight line in this diagram. Clearly the C^{18}O - A_V relation deviates from a straight line at high extinctions and N_2H^+ deviates at both high and low A_V . Such structure in this relation could be due to freeze-out/depletion or high opacities (observations of a lesser abundant isotope confirm freeze-out for CO). The various solid and dashed lines show emission profiles predicted by the chemical model for various times. As time proceeds the C^{18}O emission declines via freeze-out; in contrast the N_2H^+ emission increases (as a result of CO freeze-out). The dotted line is the “best fit” radial abundance profile which reproduces the emission profile shown as a solid line. For C^{18}O the

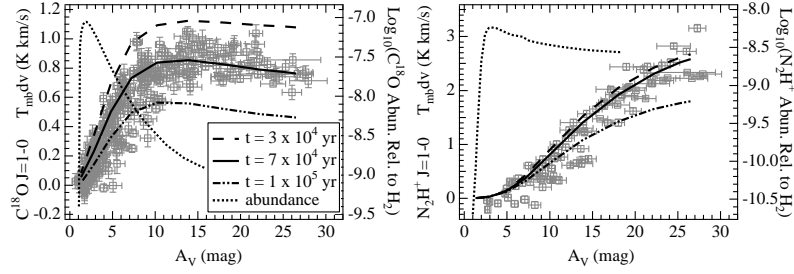


Fig. 4. Point by point comparison of C^{18}O and N_2H^+ $J=1-0$ integrated intensity with A_V the entire B68 dark cloud. In all plots the data are presented as open squares with error bars while solid curves represent the emission predicted by a model combining chemistry with a Monte-Carlo radiative transfer code. The various lines delineate the time-dependence in the chemistry. The dashed lines are the best fit molecular abundance profiles with the axis labeled to the right (abundance of N_2H^+ is multiplied by 100). Adapted from Bergin et al. (2002).

observations require significant freeze-out and also an abundance reduction at low extinction due to photo-dissociation. In the case of N_2H^+ an abundance reduction at low extinction is also required.³

B68 is just one example of a core where, using new techniques, we are inferring significant freeze-out in the early stages of star formation. Other examples can be found in the work of Tafalla et al. (2002) and references in §3. One possibility that cannot be discounted at present is that nearly all typically used molecular tracers are absent from the gas in the innermost regions of these cores (Bergin et al. 2002); this may hinder our ability to study the earliest stages star formation. However, these sources still offer great promise as new and more precise laboratories for testing chemical theory than previous work in template sources such as TMC-1 and L134N.

3.2 Chemistry in Star-Forming Cores

The chemistry in star-forming cores overlaps with the chemical studies of hot cores. Hot cores are molecular condensations directly associated with young embedded massive stars. Stellar birth leads to the creation of sharp temperature gradients and higher temperatures lead to the release of frozen ices from grain surfaces. As a result hot cores have quite different chemical composition, extending to very complex molecular species, than typically observed in quiescent gas. While these regions are associated with massive stars it is clear that low-mass stars also can produce similar “warm” cores (Cazaux et al. 2003). The reader is referred to the following references for additional discussions (Millar 2001; van der Tak 2003).

³ This is due to freeze-out of N_2 .

Examples of the new iterative method to derive abundances use so-called “jump” models where abundances are enhanced in the inner core via grain surface evaporation and are lower in the outer layers. The jump transition is set by the evaporation temperature (see van der Tak 2003). Models where chemical networks are directly linked to the radiation transport code are exemplified by the work of Doty et al. (2002) and Boonman et al. (2003).

A generic result is that enhanced abundances of numerous molecules are required in the center. A key goal for hot core studies is to probe the extent of grain surface chemistry via observations of trace complex species in the gas. Grain mantles can be observed directly via vibrational modes absorbing background IR radiation, but this method lacks sensitivity for all but the most abundant ices. Thus, gas-phase observations can be used to probe the extent of grain surface chemistry beyond the production of H_2O , CH_4 , and NH_3 . The problem is that when molecules are released from the grain they might react in the gas (Charnley, Tielens, & Millar 1992). To draw upon a parallel to cometary observations, the products of these reactions would be ion-molecule daughter products as opposed to parent molecules that have directly evaporated from the grain surface. This is further complicated by the potential presence of high temperature gas-phase chemistry. Advances in our understanding will require continued close coupling of chemical models to observations.

4 Shock Chemistry

Another area of observational astrochemistry is the evidence for shock chemistry detected in molecular outflows. The primary example is found in the highly collimated L1157 molecular outflow, which has been subjected to a detailed chemical survey (Bachiller et al 2001). This study has shown that some species have enhanced abundances in outflow lobes (SiO , CH_3OH , HCN) while others (N_2H^+ , DCO^+) are absent from the flow. Another collimated outflow, BHR71, has recently been the focus of an extensive chemical survey (shown in Figure 5). In this source the abundance trends are quite similar to L1157 in regards to the presence or absence of enhancements for most species. However, clear differences are found in the magnitude of the abundance enhancements (Bourke et al. 2004). It is not clear whether the differences are intrinsic or due to assumptions in the analysis.

Abundance enhancements are typically attributed to grain mantle core and mantle release via sputtering and/or high temperature chemistry. The effects of the latter have not been observationally explored and more attention needs to be paid to models in the literature (see series by Pineau des Forêts and collaborators). Moreover if shocks are truly liberating mantles then outflows should show high levels of deuteration as seen in hot cores. This also needs to be explored.

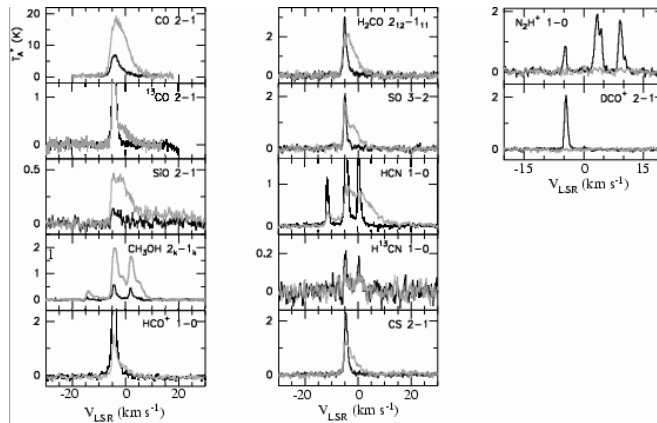


Fig. 5. Spectra of selected species taken from a chemical survey of the BHR71 outflow (Bourke et al. 2004). Dark lines indicate spectra taken towards the quiescent core while grey lines are spectra towards the peak of the red lobe of the outflow.

5 Conclusions

It is clear we are at the beginnings of a new era in astrochemistry where we will obtain more precise information regarding the abundances of molecular species, but also set limits on the abundance profile and on basic theory. In Figure 6 we present a schematic that shows a rough outline of our current understanding of the chemical structure in star forming cores. An important point here is that these zones will be different for various species (depending on the evaporation temperature, photo-dissociation cross-sections, depletion rate, etc.). Since molecular emission is the only way to probe gas kinematics, one can use improved chemical information as a tool. Thus, with careful choice of tracers, and knowledge of the chemistry, one can selectively probe motions from different gas along a given line of sight. This will be an important key to unraveling the star formation puzzle. In all, new observations are leading to crucial tests of chemical theory, but also presenting a completely new approach to star formation studies, bringing astrochemistry into wider application as a potent tool.

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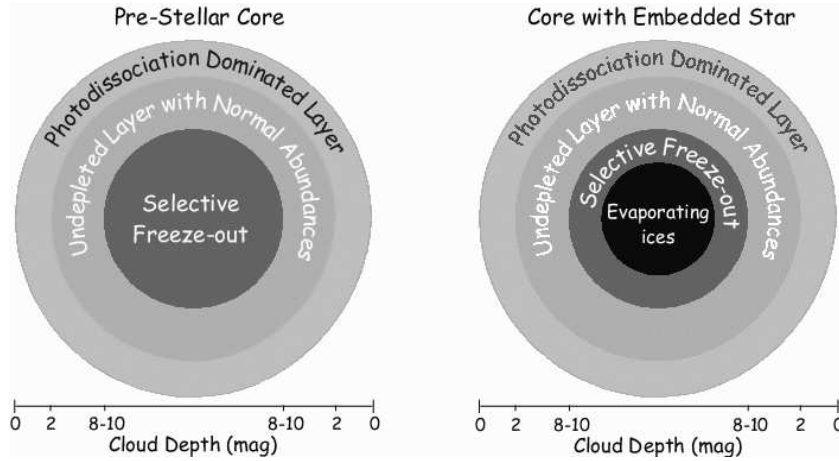


Fig. 6. Schematic of inferred chemical structure in star-forming cores. Extinction scales are calibrated to low-mass cores.

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